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VERIFICATION AND VALIDATION OF SIMULATION MODELS UNDER UNCERTAINTY

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This paper presents methodologies for validating computational models under physical, informational and model uncertainties. Integrated computational and test-based methods are being investigated at Vanderbilt University, under funding from Sandia National Laboratories, NASA, and NSF, to incorporate all three types of uncertainty for design and certification analyses of complex engineering systems. The test-only based approach is very expensive and does not make use of available analytical models of system behavior, failure modes and sensitivities. Inexpensive modeling and simulation-based methods are able to use such information. However, with the approximations in the computational models and the limited amount of statistical data on the input variables, it is difficult to associate a high degree of confidence with prediction based only on computational methods. Therefore, this paper will propose a Bayesian methodology to develop validation metrics that integrate uncertainties in both computational and empirical methods. The simulation models that we address in this paper are primarily finite element-based structural analysis and limit state-based reliability prediction models.

Verification and validation under uncertainty involves quantifying the error in the model prediction and effectively comparing the prediction with the experimental result when both prediction and test data are stochastic. Several deterministic *a posteriori* error estimates are available in the literature for adaptive mesh refinement and model verification in finite element analysis. This paper presents a method to estimate the statistical distribution of discretization error in the prediction of finite element-based computational models. A collocation-based stochastic response surface method (SRSM) is developed for computational efficiency in predicting the stochastic distribution of error. Next, a Bayesian methodology is developed for model validation. The prior distribution of error in predicting the response is first computed, which is then updated based on experimental observation using Bayesian analysis. The prior and posterior error distributions are used to compute a validation metric that judges the validity of model prediction.

Several components of computational prediction error, such as discretization error, element error, and stochastic analysis error are included. Two types of measurement error are included, in the context of model validation: error in the measurement of input variables that affects the model prediction, and error in the measurement of output variables. This paper also investigates the quantification of model form error in computational modeling and simulation under uncertainty at various stages. While methods are available to quantify model uncertainty using multiple models, this paper discusses the model form error estimation from a single model. The model form uncertainty is treated as a random variable and the statistical distribution of the model form error is then obtained by resampling the measured data repeatedly using the smoothed bootstrapping technique. Thus model error estimation requires that a sufficient number of test results are available to construct the probability density function.

This paper explores the error combination method in model validation, addressing various types of uncertainties and errors in both computational predictions and validation experiments. The proposed error combination method is based on the construction of a response surface for total error or observed error in terms of all the error components which are treated as random variables. Based on a validation metric, error and uncertainty quantification can provide a quantitative means for judging whether the model is sufficiently accurate or in need of refinement and then permits trade off between computational effort and experimental effort. The sensitivity analysis facilitates refinements in data collection for input and output variables, mathematical model, numerical model (e.g., FEM mesh), and uncertainty propagation model.

The concept of Bayesian hypothesis testing is extended to system-level problems where full-scale testing is impossible. Component-level validation results are used to derive a system-level validation measure. This derivation depends on the knowledge of inter-relationships between component modules. Bayes networks are used for the propagation of validation information from the component-level to system-level. Markov Chain Monte Carlo techniques aid in updating the statistical distributions of component level response and hence the system level response. The computational method is illustrated with a numerical example involving reliability prediction of a single degree of freedom turbine engine blade under high-cycle fatigue. The limit state function is treated as a system level response while dynamic parameters and mechanical parameters are treated as subsystems and components having validation data.

A computational model may generate multiple response quantities at a single location or the same response quantity at multiple locations, and a validation experiment might yield corresponding measured responses in a single test. In each case, the multiple responses, being derived from same input, are correlated and model validation involves comparison of joint probability densities of model prediction and test data (multivariate analysis). The Bayesian validation metric proposed for comparing a single prediction with a single observation will be extended for this purpose. Also, each decision variable can be validated individually or a collective metric can be developed to validate the correlated quantities in order to judge the overall performance of the code. The proposed concept is applied to a problem involving shock physics and wave propagation in two colliding solid aluminum plates. The shock wave velocities for different levels of momentum are predicted by an empirical model and validated against some observations.

In particular cases, validation of statistical model or distribution may be of concern instead of a single prediction values. One has to verify that the available data belongs to distribution predicted by the model. In such situations, the first two moments of probability density functions of the response obtained from model and data are compared. While classical hypothesis test methods fail to reject a wrong model (Type II error), the Bayesian hypothesis testing provides a rational validation process. The proposed method is illustrated for a practical problem involving mechanical properties of joints found in weapons systems and their structural response under dynamic loading. Quasi-Static mathematical models with uncertain parameters are built to explain the dissipative mechanism of lap joints and such empirical models are validated against experimental data.

One problem in practical application is to extend what we can learn about the model's predictive capability within the tested region to an inference about the predictive capability in the application or untested region. Confidence in the prediction near off-nominal region by a model, already validated in the nominal region, needs to be quantified. One approach is to construct a regression model for the test data in the validation domain, and to simulate test data in the untested region using this model. Inferences may be made in an incremental fashion from validation region to untested region, aided by bootstrapping and cross validation.

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